Supplementary Information

Novel anti-Prelog stereospecific carbonyl reductases from *Candida parapsilosis* for asymmetric reduction of prochiral ketones

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1. Settings of grid box dimensions and centers in flexible docking

All docking calculations were accomplished with AutoDock Vina 1.0. A docking algorithm that took account of ligand flexibility but kept the protein rigid was employed. Docking runs were carried out using the standard parameters of the program for interactive growing and subsequent scoring, except for the parameters for setting grid box dimensions and center. The values for setting grid box dimensions and centers in docking studies are as follows.

1.1 Grid options for enzyme-NADPH docking
receptor = scr.pdbqt
ligand = nadph.pdbqt
center_x = -8.558
center_y = 5.024
center_z = -3.026
size_x = 20
size_y = 22
size_z = 20

1.2 Grid options for enzyme-NADH docking
receptor = scr.pdbqt
ligand = nadh.pdbqt
center_x = -8.558
center_y = 5.024
center_z = -3.026
size_x = 20
size_y = 22
size_z = 20

1.3 Grid options for enzyme-cofactor-substrate docking
receptor = scr-nadph.pdbqt
ligand = cobe.pdbqt
center_x = -17.447
center_y = 15.961
center_z = -9.463
size_x = 18
size_y = 20
size_z = 22

Analytic methods for different kinds of chiral alcohol products

The reaction products were analyzed by chiral HPLC (HP 1100, Agilent, USA) equipped with Chiralcel OB-H column (4.6 mm × 250 mm; Daicel Chemical Ind. Ltd., Japan), or chiral GC (7890A, Agilent, USA) equipped with FID detector and Chrompack Chirasil-Dex CB chiral capillary column (25 m × 0.25 mm; Varian, USA). The product configuration of aryl alcohols and hydroxyl esters was measured by HPLC with a Chiralcel OB-H column (4.6 × 250 mm) at 30 ^{o}C, eluted with hexane/2-propanol (90:10 or 95:5 or 98:2, v/v) at 0.5 ml/min, and detected at 215 nm. The product configuration of aliphatic alcohols was determined by the derivation of alcohols. (R)-PEIC (10 μl) was added to the dried sample of alcohol in nonane (100 μl). After 45 min at 37 ^{o}C, ethanol (20 μl) was added to stop the derivation and the products were analyzed by GC on column Chrompack Chirasil-Dex CB (25 m × 0.25 mm, 1 bar H_2) using the following temperature program: 120 ^{o}C/2 min–10 ^{o}C/min–200 ^{o}C/5 min. Absolute configurations of chiral alcohol products were determined by comparison of elution order on HPLC or GC with published data,[2,3,4,5] or co-injection with commercial available materials.

References

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1H NMR spectrum of 1-phenyl-1,2-ethanediol

^{1}H NMR analysis of the reaction product of 1-phenyl-1,2-ethanediol was carried out on a Varian Unity-400 MHz spectrometer (400MHz, $CDCl_3$).